

10 10

=> d his

(FILE 'HOME' ENTERED AT 09:41:10 ON 17 AUG 2005)

FILE 'REGISTRY' ENTERED AT 09:41:47 ON 17 AUG 2005

L1 STRUCTURE uploaded
L2 0 S L1 CSS
L3 43 S L1
L4 1056 S L1 FUL

FILE 'CAPLUS' ENTERED AT 09:43:18 ON 17 AUG 2005

L5 516 S L4
L6 102044 S DIABETES
L7 11 S L6 AND L5
L8 STRUCTURE uploaded
S L8

FILE 'REGISTRY' ENTERED AT 09:47:30 ON 17 AUG 2005

L9 25 S L8

FILE 'CAPLUS' ENTERED AT 09:47:30 ON 17 AUG 2005

L10 29 S L9

FILE 'REGISTRY' ENTERED AT 09:47:38 ON 17 AUG 2005

L11 663 SEARCH L8 SSS SUB=L4 FUL

FILE 'CAPLUS' ENTERED AT 09:48:13 ON 17 AUG 2005

L12 338 S L11
L13 11 S L12 AND L6

FILE 'REGISTRY' ENTERED AT 09:48:58 ON 17 AUG 2005

L14 15 S L8 CSS FUL

FILE 'CAPLUS' ENTERED AT 09:49:52 ON 17 AUG 2005

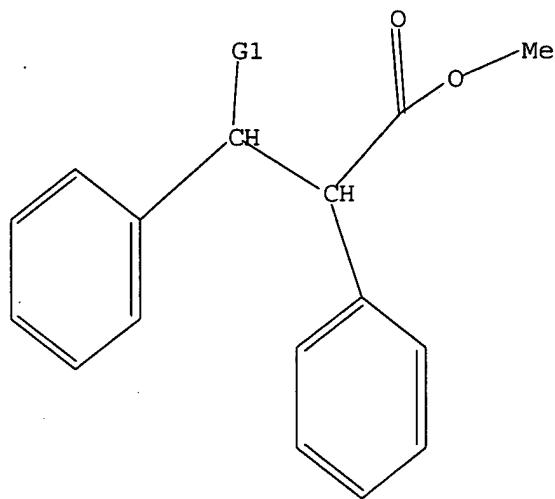
L15 58 S L14

FILE 'USPATFULL' ENTERED AT 09:50:01 ON 17 AUG 2005

L16 4 S L15

FILE 'CAPLUS' ENTERED AT 09:51:01 ON 17 AUG 2005

=> d 18
L8 HAS NO ANSWERS
L8 STR



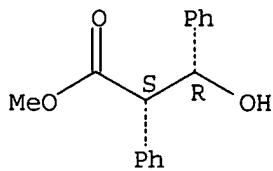
G1 H,Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,OH

Structure attributes must be viewed using STN Express query preparation.

=> d bib abs hitstr 35-58 115

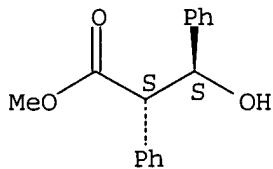
L15 ANSWER 35 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1982:169662 CAPLUS
 DN 96:169662
 TI Effect of shift reagents on infrared spectra
 AU Porter, Geoffrey B.; Simpson, Jon
 CS Dep. Chem. Metall., R. Mil. Coll. Sci., Shrivenham/Swindon/Wilts., SN6
 8LA, UK
 SO Spectroscopy Letters (1981), 14(11-12), 755-61
 CODEN: SPLEBX; ISSN: 0038-7010
 DT Journal
 LA English
 AB The IR spectra of Eu(fod)₃ shift reagent (Hfod = 6,6,7,7,8,8,8-heptafluoro-2,2-dimethyl-3,5-octanedione) were determined in CCl₄ solns. containing Me threo- and erythro-2,3-diphenyl-3-hydroxypropanoate, Me 2-phenylethanoate, and 2-butanone at 25°. An adsorption at 1690 cm⁻¹ is due to CO-Eu interaction. Equilibrium consts. were calculated from peak areas by assuming 1:1 interaction. The pK values are 3.7, 3.6, 2.4, and 2.9 ± 0.1, resp. The OH group reinforces CO interaction via a chelate effect.
 IT 17226-93-6DP, europium shift reagent complexes
 17226-94-7DP, europium shift reagent complexes
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, in carbon tetrachloride, IR spectral study of)
 RN 17226-93-6 CAPLUS
 CN Benzenepropanoic acid, β-hydroxy-α-phenyl-, methyl ester,
 (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



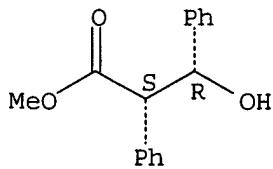
RN 17226-94-7 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



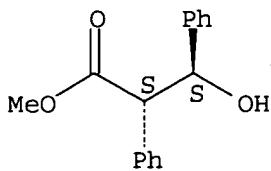
L15 ANSWER 36 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1980:532206 CAPLUS
 DN 93:132206
 TI Effect of the type of base on the yield and stereoselectivity of the low-temperature Claisen reaction. II. Experiments with alkali metals
 AU Krachanov, Kh.; Kirchev, N.; Kurtev, B.
 CS Vissch Inst. Khranitel. Vkusova Prom., Plovdiv, Bulg.
 SO Nauchni Trudove - Vissch Institut po Khranitelna i Vkusova Promishlenost, Plovdiv (1978), 25, Pt. 1, 333-5
 CODEN: NTKVAH; ISSN: 0477-0250
 DT Journal
 LA Bulgarian
 AB The catalytic activity of alkali metals in Claisen condensation of PhCH₂CO₂Me with PhCHO increased in the order Li < Na < K. HOCHPhCHPhCO₂Me was formed in 72 and 84% yield and 4:1 and 2.8:1 threo-erythro ratio with Na and K, resp.
 IT 17226-93-6P 17226-94-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 17226-93-6 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



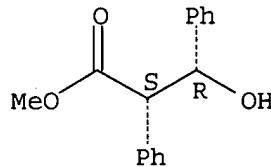
RN 17226-94-7 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



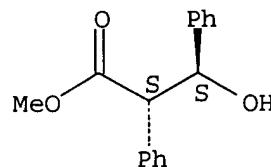
L15 ANSWER 37 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1980:76060 CAPLUS
 DN 92:76060
 TI Stereoselective synthesis of β -hydroxy esters by low-temperature Claisen reaction. IV. Effect of base on the yield and stereoselectivity of the reaction in ether
 AU Krachanov, Kh.; Kirchev, N.; Kurtev, B.
 CS Vissch Inst. Khranitel. Vkusova Prom., Plovdiv, Bulg.
 SO Izvestiya po Khimiya (1979), 12(1), 3-7
 CODEN: IZKHDX; ISSN: 0324-0401
 DT Journal
 LA German
 AB The Claisen condensation of BzH with $\text{PhCH}_2\text{CO}_2\text{Me}$ (I) was studied in ether at -24° in the presence alkali metal amides and ethoxides. The best yields and stereoselectivity for threo- $\text{HOCHPhCHPhCO}_2\text{Me}$ were achieved using NaNH_2 in amts. equivalent to that of I.
 IT 17226-93-6P 17226-94-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 17226-93-6 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 17226-94-7 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β R)-rel- (9CI) (CA INDEX NAME)

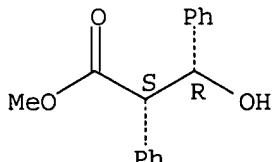
Relative stereochemistry.



L15 ANSWER 38 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1978:529206 CAPLUS
 DN 89:129206

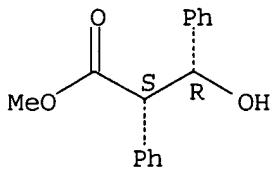
TI Interaction of substituted benzaldehydes with methylphenylacetate during low-temperature Claisen reaction
 AU Kirchev, N.; Krachanov, Kh.
 CS Inst. Food Technol., Plovdiv, Bulg.
 SO Doklady Bolgarskoi Akademii Nauk (1978), 31(1), 59-61
 CODEN: DBANAD; ISSN: 0366-8681
 DT Journal
 LA English
 AB Reaction of $\text{PhCH}_2\text{CO}_2\text{Me}$ with $\text{RnC}_6\text{H}_5\text{-nCHO}$ ($\text{Rn} = \text{H, 2-F, 2-Cl, 3-Cl, 2,6-Cl}_2$, 3-Me, 4-MeO, etc.) in Et_2O at -24° for 2 h in the presence of NaNH_2 stopped at the aldol stage and gave eighteen $\text{RnC}_6\text{H}_5\text{-nCH(OH)CHPhCO}_2\text{Me}$ (I) in 31-85% yield, with threo/erythro ratio in the product varying from 96:4 to 69:31. There was no well-defined relation between the nature and position of the substituent and the yield of I.
 IT 17226-93-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 17226-93-6 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 ($\alpha\text{R},\beta\text{S}$)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



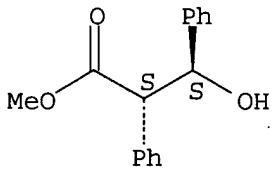
L15 ANSWER 39 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1978:104853 CAPLUS
 DN 88:104853
 TI Stability of diastereomeric 2,3-diphenyl-3-hydroxypropanoic acids and their esters during heating in triethylamine medium
 AU Kirchev, N.; Krachanov, Kh.
 CS Vissch Inst. Khranit. Vkusova Prom., Plovdiv, Bulg.
 SO Nauchni Trudove - Vissch Institut po Khranitelna i Vkusova Promishlenost, Plovdiv (1976), 23(3), 139-46
 CODEN: NTKVAH; ISSN: 0477-0250
 DT Journal
 LA Bulgarian
 AB Diastereoisomeric $\text{ROCHPhCHPhCO}_2\text{R}_1$ (I; $\text{R} = \text{R}_1 = \text{H}$; $\text{R} = \text{H, Ac, R}_1 = \text{Me}$) were stable toward Et_3N at room temperature in the presence or absence of $(\text{Me}_2\text{N})_3\text{PO}$, but underwent retro-aldol decomposition at 80° in the presence of $(\text{Me}_2\text{N})_3\text{PO}$. The stability of the acid exceeded that of the esters. No significant isomerization of I was observed. Condensation reaction of $\text{PhCH}_2\text{CO}_2\text{Me}$ with PhCHO in the presence of Et_3N at -24 to $+80^\circ$ afforded threo- and erythro-I ($\text{R} = \text{H, R}_1 = \text{Me}$) in 1:2 ratio and $\leq 5\%$ combined yield.
 IT 17226-93-6 17226-94-7
 RL: PRP (Properties)
 (stability of, to isomerization and retro-aldol decomposition)
 RN 17226-93-6 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 ($\alpha\text{R},\beta\text{S}$)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



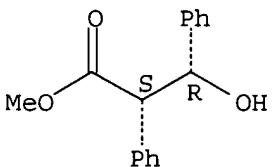
RN 17226-94-7 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



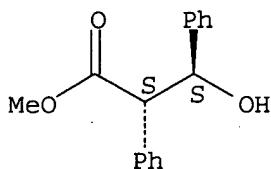
L15 ANSWER 40 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1978:67547 CAPLUS
 DN 88:67547
 TI Effect of shift reagents on NMR coupling constants
 AU Porter, Geoffrey Brian; Simpson, Jon
 CS Chem. Branch, R. Mil. Coll. Sci., Shrivenham/Swindon, UK
 SO Angewandte Chemie (1978), 90(1), 51-2
 CODEN: ANCEAD; ISSN: 0044-8249
 DT Journal
 LA German
 AB A significant effect is reported of the NMR shift reagents [D27]-Eu(fod)3 and [D27]-La(fod)3 (Hfod = F3C(CF2)2COCH2COCMe3) on the J values for vicinal coupling of esters of 2,3-diphenyl-3-hydroxypropionic acid in 1H NMR. After the addition of the shift reagents the chemical shift of the 1H NMR signal indicates the formation of a 1:1 complex. The data can be interpreted in terms of chelate formation of the potentially 2-coordinating hydroxy esters, whereby both functional groups are in the gauche position.
 IT 17226-93-6 17226-94-7
 RL: PRP (Properties)
 (NMR coupling consts. of, lanthanide shift reagent effects on)
 RN 17226-93-6 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



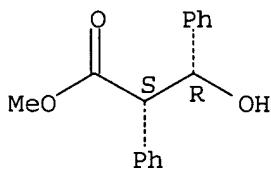
RN 17226-94-7 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



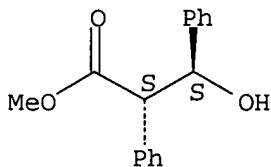
L15 ANSWER 41 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1977:105406 CAPLUS
 DN 86:105406
 TI Stereoselective synthesis of β -hydroxy esters via the low-temperature Claisen reaction
 AU Krachanov, Kh.; Kirchev, N.; Kurtev, B.
 CS Higher Inst. Food Technol., Plovdiv, Bulg.
 SO Izvestiya po Khimiya (1976), 9(2), 338-47
 CODEN: IZKHDX; ISSN: 0324-0401
 DT Journal
 LA English
 AB The condensation of PhCHO with PhCH₂CO₂R (R = Me, Et, Pr, CHMe₂, Bu, CMe₃) in Et₂O at low temps. (.apprx.-20°) in the presence of NaNH₂ gave 78% of the threo isomer of PhCH(OH)CHPhCO₂R. The stereoselectivity is under thermodn. control. Catalytic amts. of NaNH₂ lower the yields and stereoselectivity slightly.
 IT 17226-93-6P 17226-94-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 17226-93-6 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



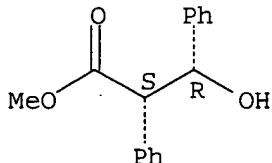
RN 17226-94-7 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



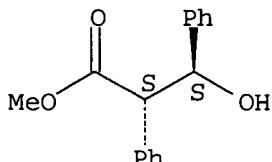
AN 1976:477455 CAPLUS
 DN 85:77455
 TI Effect of substituents on the stereochemistry of the Reformatskii reaction
 AU Mladenova, M.; Blagoev, B.; Kurtev, B.
 CS Inst. Org. Chem., Sofia, Bulg.
 SO Doklady Bolgarskoi Akademii Nauk (1975), 28(12), 1633-6
 CODEN: DBANAD; ISSN: 0366-8681
 DT Journal
 LA French
 AB The Reformatskii reaction of RC_6H_4CHO ($R = H, p\text{-Me}, o\text{-Me}, p\text{-Cl}, o\text{-Cl}, p\text{-MeO}$) and 1-naphthaldehyde with $p\text{-R}_1C_6H_4CHBrCO_2Me$ ($R_1 = Br, H$) gave an apprx. 50:50 mixture of erythro- and threo- $RC_6H_4CH(OH)CH(C_6H_4R_1-p)CO_2Me$ or the 1-naphthyl analog in Et_2O . In $(MeO)_2CH_2$, the erythro isomer was slightly favored (apprx. 60:40); in Me_2SO , the threo isomer was favored (apprx. 70:30). In Me_2SO , $p\text{-R}_1C_6H_4CH(CO_2Me)CH(CO_2Me)C_6H_4R-p$ was also formed. The lack of substituent effects in the Reformatskii reaction was explained by a transition state resembling the starting materials.
 IT 17226-93-6P 17226-94-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 17226-93-6 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 ($\alpha R, \beta S$) -rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 17226-94-7 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 ($\alpha R, \beta R$) -rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L15 ANSWER 43 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1976:121375 CAPLUS
 DN 84:121375
 TI Absolute configurations of the diastereomeric 3-hydroxy-2,3-diphenylpropanoic acids.
 AU Berova, N.; Kurtev, B.
 CS Inst. Org. Chem., Sofia, Bulg.
 SO Izvestiya po Khimiya (1975), 8(1), 77-83
 CODEN: IZKHDZ; ISSN: 0324-0401
 DT Journal
 LA English
 AB Chemical correlation with enantiomeric Me 2,3-diphenylpropanoates showed that

(-) -erythro- and (+) -threo-3-hydroxy-2,3-diphenylpropionic acid have the S,S and 2R,3S configurations, resp.

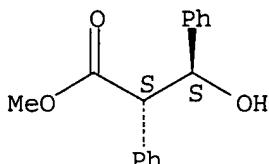
IT 58769-52-1P 58769-53-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

RN 58769-52-1 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
[S-(R*,R*)]- (9CI) (CA INDEX NAME)

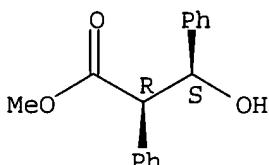
Absolute stereochemistry.



RN 58769-53-2 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
[S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



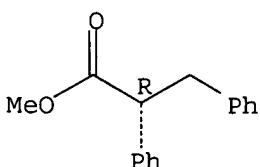
IT 58714-10-6P 58714-11-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 58714-10-6 CAPLUS

CN Benzenepropanoic acid, α -phenyl-, methyl ester, (α R)- (9CI)
(CA INDEX NAME)

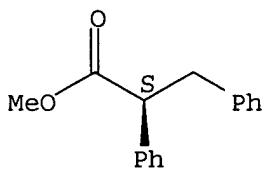
Absolute stereochemistry. Rotation (-).



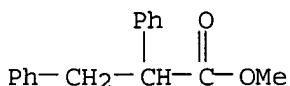
RN 58714-11-7 CAPLUS

CN Benzenepropanoic acid, α -phenyl-, methyl ester, (α S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 44 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1976:89550 CAPLUS
 DN 84:89550
 TI Diacids and α,α -disubstituted mixed functional acids and their derivatives. XLIV-Chain-ring isomerism of some γ -aldehydic acids and disubstituted α -gem-succinic aldehyde esters. Application to the selective reaction of nucleophiles
 AU Des Abbayes, Herve; Neveu, Cecile; Salmon-Legagneur, Francois
 CS Dep. Phys. Crist. Chim. Struct., Univ. Rennes, Rennes, Fr.
 SO Bulletin de la Societe Chimique de France (1973), (9-10, Pt. 2), 2686-92
 CODEN: BSCFAS; ISSN: 0037-8968
 DT Journal
 LA French
 OS CASREACT 84:89550
 GI For diagram(s), see printed CA Issue.
 AB The open and closed isomers, $\text{HCOCH}_2\text{CRR}_1\text{CO}_2\text{H}$ (I, R = R1 = Me; R = Ph, R1 = Me, Ph, PhCH_2) and II (R, R1 have same meaning), from the ring-chain isomerization of I were blocked by methylation, which gave the Me ester (III) of I and the O-Me derivative (IV) of II and permitted selective reaction with nucleophiles. Thus, I were quant. converted by MeMgI into valerolactones (V, R2 = Me) (VI); VI were also obtained, in some cases, by the reaction of MeMgI with III, but reaction of MeMgI with IV gave $\text{MeOCH}_2\text{CRR}_1\text{CO}_2\text{H}$. Reaction of I with morpholine gave V (R2 = morpholino), III gave ester enamines $\text{R}_2\text{NCH}=\text{CHCRR}_1\text{CO}_2\text{Me}$ (R, R1 same as in I, R2N = morpholino), and IV did not react. The mechanisms of the reactions are discussed.
 IT 35030-49-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with bromoacetaldehyde acetal)
 RN 35030-49-0 CAPLUS
 CN Benzenepropanoic acid, α -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L15 ANSWER 45 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1975:125008 CAPLUS
 DN 82:125008
 TI Application of the low temperature Claisen reaction for stereoselective synthesis of threo-3-aryl-3-hydroxy-2-phenylpropanoic acids and their methyl esters
 AU Kurtev, B.; Kratchanov, Kh.; Kirchev, N.
 CS Inst. Org. Chem., Sofia, Bulg.
 SO Synthesis (1975), (2), 106-8
 CODEN: SYNTBF; ISSN: 0039-7881
 DT Journal
 LA English

OS CASREACT 82:125008

AB RCHO (R = Ph, 4-FC6H4, 2-, 3-, 4-ClC6H4, 2,6-Cl2C6H3, 2- and 4-BrC6H4) condensed with PhCH2CO2R1 (R1 = Me, CMe3) at -24° in Et2O or (Me2CH)2O containing NaNH2 gave threo-HOCHRCHPhCO2R1 (I) in 40-85% yield from the solid phase of the reaction mixture; I (R = Ph, R1 = CM3) was hydrolyzed to I (R = Ph, R1 = H) in 93% yield by heating with CF3CO2H. The I yield was lower and the erythro-threo ratio was higher in different solvents or with NaOEt instead of NaNH2.

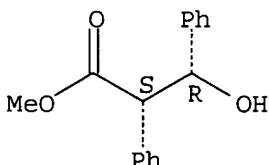
IT 17226-93-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 17226-93-6 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L15 ANSWER 46 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1975:30853 CAPLUS

DN 82:30853

TI Stereochemistry of the Reformatsky reaction

AU Mladenova, M.; Blagoev, B.; Kurtev, B.

CS Inst. Org. Chim., Sofia, Bulg.

SO Bulletin de la Societe Chimique de France (1974), 7-8, Pt. 2, 1464-8
CODEN: BSCFAS; ISSN: 0037-8968

DT Journal

LA French

AB The effect of solvent, temperature, alkyl group (R) and metal (Zn, Mg) on the stereochem. and the reversibility of the Reformatskii reaction of PhCHBrCO2R (R = Me, CHMe2 and CMe3) with BzH was investigated.

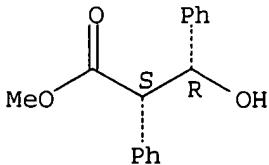
IT 17226-93-6P 17226-94-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 17226-93-6 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β S)-rel- (9CI) (CA INDEX NAME)

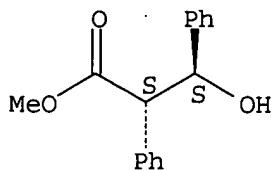
Relative stereochemistry.



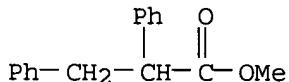
RN 17226-94-7 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β R)-rel- (9CI) (CA INDEX NAME)

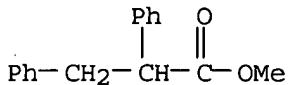
Relative stereochemistry.



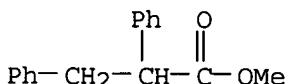
L15 ANSWER 47 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1974:463032 CAPLUS
 DN 81:63032
 TI NMR spectra and conformation of 1,2-diphenylpropane and 2,3-diphenylpropanoic acid
 AU Spassov, S. L.; Orahovats, A. S.; Mishev, S. M.; Schraml, J.
 CS Inst. Org. Chem., Bulg. Acad. Sci., Sofia, Bulg.
 SO Tetrahedron (1974), 30(2), 365-8
 CODEN: TETRAB; ISSN: 0040-4020
 DT Journal
 LA English
 AB NMR spectra of $\text{PhCH}_2\text{CHPhR}$ ($= \text{R Me, CO}_2\text{H, CO}_2\text{Me}$) and deuterated analogs showed the predominance of the conformer with anti-periplanar Ph groups. The values of the gauche nonbonded interaction energies ($-\Delta E$ kcal/mole) are 0.8 for Ph/Ph, 0.6 for Ph/CO₂H, and 0.4 for Ph/CO₂Me.
 IT 35030-49-0
 RL: PRP (Properties)
 (conformation of, NMR in relation to)
 RN 35030-49-0 CAPLUS
 CN Benzenepropanoic acid, α -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L15 ANSWER 48 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1973:485283 CAPLUS
 DN 79:85283
 TI Constitution dependence and the benzene induced effect of the chemical shifts of some carboxylic acid methyl ester methoxy protons
 AU Brink, Maud; Larsson, Erik
 CS Chem. Inst., Univ. Lund, Lund, Swed.
 SO Organic Magnetic Resonance (1973), 5(7), 327-31
 CODEN: ORMRBD; ISSN: 0030-4921
 DT Journal
 LA English
 AB The chemical shifts of the MeO protons in .apprx.60 Me esters of carboxylic acids were obtained in CCl₄ and C₆D₆, and their dependence on constitution and solvent are discussed. The values of a certain mol. could be assumed to be composed additively of a number of parameters which characterize the substituents.
 IT 35030-49-0
 RL: PRP (Properties)
 (NMR of)
 RN 35030-49-0 CAPLUS
 CN Benzenepropanoic acid, α -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L15 ANSWER 49 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1973:110782 CAPLUS
 DN 78:110782
 TI Thallium in organic synthesis. XXXIV. Oxidations of acetylenes with thallium(III) nitrate (TTN)
 AU McKillop, Alexander; Oldenziel, Otto H.; Swann, Brian P.; Taylor, Edward C.; Robey, Roger L.
 CS Sch. Chem. Sci., Univ. East Anglia, Norwich/Norfolk, UK
 SO Journal of the American Chemical Society (1973), 95(4), 1296-301
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal
 LA English
 AB The reactions of a variety of acetylenes with thallium(III) nitrate (TTN) have been examined, and the nature of the products has been found to depend on the solvent employed and the structure of the acetylene. Diarylacetylenes are converted into benzils in high yields on treatment with TTN in either aqueous acidic glyme or in MeOH; dialkylacetylenes gives acyloins in aqueous media and α -methoxy ketones in MeOH; monoalkylacetylenes undergo degradation to carboxylic acids containing one C atom less than the starting material; and alkylarylacetylenes undergo smooth oxidative rearrangement in MeOH solution to give methyl α -alkylarylacetates. All of the reactions proceed in high yield, and the specificity in oxidation is explained in terms of the mechanisms of the various reactions. Hydration of the C.tpbond.C bond does not occur to a significant extent.
 IT 35030-49-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 35030-49-0 CAPLUS
 CN Benzenepropanoic acid, α -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L15 ANSWER 50 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1972:45888 CAPLUS
 DN 76:45888
 TI Thallium in organic synthesis. XXVIII. Selective oxidation of acetylenes to carboxylic acids, acyloins, benzils, and arylacetic acids with thallium(III) nitrate
 AU McKillop, Alexander; Oldenziel, Otto H.; Swann, Brian P.; Taylor, Edward C.; Robey, Roger L.
 CS Sch. Chem. Sci., Univ. East Anglia, Norwich/Norfolk, UK
 SO Journal of the American Chemical Society (1971), 93(26), 7331-3
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal
 LA English
 AB Reactions of a variety of acetylenes with thallium(III) nitrate were

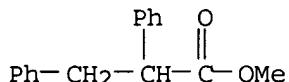
examined Diarylacetylenes may be converted into benzils in high yield, dialkylacetylenes give acyloins, monoalkylacetylenes undergo degradation to carboxylic acids containing 1 C atom less than the starting material, and alkylarylacetylenes undergo smooth oxidative rearrangement (in MeOH) to give Me α -alkylarylacetates. All reactions proceed in high yield; the specificity in oxidation is explained in terms of the mechanisms of the various reactions. Hydration of the C.tplbond.C bond does not occur to a significant extent.

IT 35030-49-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35030-49-0 CAPLUS

CN Benzenepropanoic acid, α -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L15 ANSWER 51 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1971:476002 CAPLUS

DN 75:76002

TI Internal solvation effects on the conformation of acyclics

AU Auerbach, R. A.; Kingsbury, C. A.

CS Dep. Chem., Univ. Nebraska, Lincoln, NE, USA

SO Tetrahedron (1971), 27(11), 2069-77

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

AB Expts. attempting to discern internal solvation (or H-bonding) of CO₂H or CO₂⁻ by OH are outlined. In aqueous solns. little evidence for internal solvation exists. In basic MeOH this effect appears due to poor solvation by the solvent. The origin of anomalous coupling consts. in Me₃C compds. is discussed.

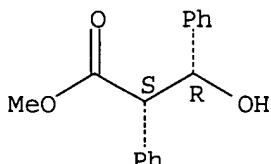
IT 17226-93-6 17226-94-7

RL: PRP (Properties)
(conformation of, N.M.R. in relation to)

RN 17226-93-6 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β S)-rel- (9CI) (CA INDEX NAME)

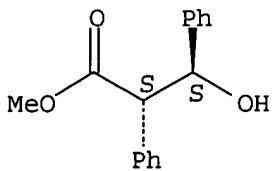
Relative stereochemistry.



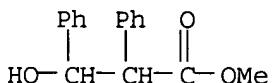
RN 17226-94-7 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L15 ANSWER 52 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1971:435343 CAPLUS
 DN 75:35343
 TI Reformatsky reaction. Threo-erythro equilibration of bromozinc alkoxides
 AU Bellassoued, Moncef; Couffignal, Rene; Gaudemar, Marcel
 CS Lab. Synth. Organomet., Univ. Paris, Paris, Fr.
 SO Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences
 Chimiques (1971), 272(19), 1686-9
 CODEN: CHDCAQ; ISSN: 0567-6541
 DT Journal
 LA French
 AB Erythro-threo mixts. of PhCR1(OZnBr)CHEtCO2R2 (I) (R1 = H and R2 = Pr)
 (II) and I (R1 = Me, R2 = Et) (III) in different ratios were prepared by
 treating the hydroxy esters with BrZnCH2CO2Et or by Reformatskii synthesis
 from PhCOR1 and BrZnCHEtCO2R2. In CH2(OMe)2 or Me2SO at -5° or
 45° for 0.5-6 hr, the mixture of secondary alcoholates of II did not
 equilibrate; the III mixture (tertiary alcoholates), prepared by the 2nd
 method, equilibrated slowly at 45° in Me2SO, but not at
 -10°. Thus, the Reformatskii reaction at low temperature is kinetically
 controlled.
 IT 93434-58-3DP, Hydracrylic acid, 2,3-diphenyl-, methyl ester, zinc
 complexes
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 93434-58-3 CAPLUS
 CN Benzenepropanoic acid, β-hydroxy-α-phenyl-, methyl ester (9CI)
 (CA INDEX NAME)



L15 ANSWER 53 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1971:405086 CAPLUS
 DN 75:5086
 TI Thin-layer chromatography on silica gel as a method for assigning the
 relative configurations to some aliphatic diastereomeric compounds
 AU Palamareva, M.; Khaimova, M.; Stefanovski, Yu.; Viteva, L.; Kurtev, B.
 CS Dep. Chem., Univ. Sofia, Sofia, Bulg.
 SO Journal of Chromatography (1971), 54(3), 383-91
 CODEN: JOCRAM; ISSN: 0021-9673
 DT Journal
 LA English
 AB The configurations of the diastereoisomeric compds. RCH(X)CH(Y)R' (X and Y
 are polar substituents and R and R' are Ph or m,p-dialkoxyphenyl) can be
 determined by thin-layer chromatog. on silica gel. The erythro isomer always
 exhibits a higher Rf value than the threo isomer, regardless of the
 developing solvent polarity of the formation of an intramol. H-bond
 between X and Y. Rf data are given for 37 diastereoisomeric pairs, and

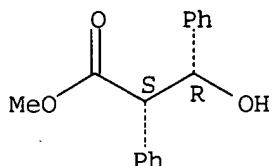
the chromatog. behavior of the compds. is explained on the basis of the preferred conformations of the isomers. The compds. were detected either with Dragendorff reagent and Et₂O-iodine or with H₂SO₄.

IT 17226-93-6 17226-94-7
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, thin-layer)

RN 17226-93-6 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β S)-rel- (9CI) (CA INDEX NAME)

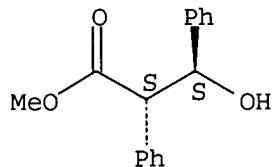
Relative stereochemistry.



RN 17226-94-7 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L15 ANSWER 54 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1969:476047 CAPLUS

DN 71:76047

TI Nuclear magnetic resonance spectra, configuration and conformation of diastereomers 3-substituted 2,3-diphenylpropanoic acids and their methyl esters

AU Spasov, Stefan L.

CS Inst. Org. Chem., Sofia, Bulg.

SO Tetrahedron (1969), 25(16), 3631-38

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

AB The N.M.R. spectra of the erythro and threo forms of compds. of the type PhCHAXCHBPhCO₂R, where X = OH, OAc, NH₂, NHMe, NHPH, NHCONH₂, NHCONHAc, and R = H or Me, have been investigated in CDCl₃ and (CD₃)₂SO solns. at normal and in some cases also at higher temperature. The values of the vicinal coupling constant J_{AB} are used to study the conformational equilibrium of the erythro and threo forms and its dependence on the solvent and temperature. The chemical-shift difference and the shape of the signals of some proton groups as R = Me and Ph are criteria permitting an unequivocal assignment of relative configuration of diastereomers of such type as well as their quant. determination in complex mixts.

IT 17226-93-6 17226-94-7

RL: PRP (Properties)

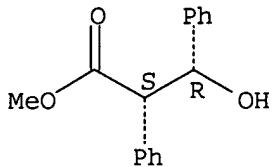
(nuclear magnetic resonance of)

RN 17226-93-6 CAPLUS

10/446,319

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β S)-rel- (9CI) (CA INDEX NAME)

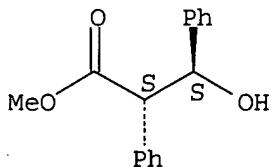
Relative stereochemistry.



RN 17226-94-7 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L15 ANSWER 55 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1967:481706 CAPLUS

DN 67:81706

TI Stereochemistry of the Reformatskii reaction. II. Ir and N.M.R. spectra of β -hydroxy esters formed. Determination of their mixtures.

Results

AU Canceill, Josette; Basselier, Jean J.; Jacques, Jean

CS College de France, Paris, Fr.

SO Bulletin de la Societe Chimique de France (1967), (3), 1024-30

CODEN: BSCFAS; ISSN: 0037-8968

DT Journal

LA French

GI For diagram(s), see printed CA Issue.

AB cf. CA 66: 28487a. An ir and N.M.R. determination of the configuration of diastereoisomers of β -hydroxy esters (I and II) from the Reformatskii reaction of ArRCO with an α -halo ester BrR₁CHCO₂R₂ led to a discussion of the influence of chelation through intramol. H bonding and steric interactions in the conformational equilibrium of these compds. Risks are involved in the generalization of results of these spectroscopic methods applied to such problems. threo- and erythro-Hydroxy esters derived from benzaldehyde (I and II, R = H) and from aromatic ketones (R different from H) are discussed and the yields are tabulated. The preps. have been described (loc. cit.).

IT 17226-93-6 17226-94-7

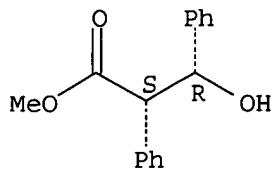
RL: PRP (Properties)

(configuration of, N.M.R. in relation to)

RN 17226-93-6 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β S)-rel- (9CI) (CA INDEX NAME)

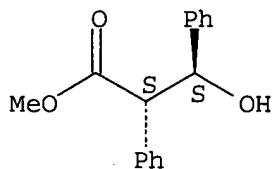
Relative stereochemistry.



RN 17226-94-7 CAPLUS

CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L15 ANSWER 56 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1963:481853 CAPLUS

DN 59:81853

OREF 59:15146f-h

TI Stereochemistry of the Reformatskii reaction

AU Canceill, Josette; Basselier, Jean Jacques; Jacques, Jean

CS College de France, Paris

SO Bulletin de la Societe Chimique de France (1963), (8-9), 1906-8

CODEN: BSCFAS; ISSN: 0037-8968

DT Journal

LA Unavailable

AB The stereochemistry of the Reformatskii reaction between PhCHO and BrCH₂CO₂R' was studied. The following PhCH(OH)CH₂CO₂R' were formed (R, R', % threo-compound in the mixture, m.p. of threo-compound, %

erythro-compound in the mixture, % yield of the reaction, and b.p. of the reaction mixture given):
 Me, Me (I), 37 \pm 5, 48-50°, 63 \pm 5, 82, b₃ 122-7°; Et,
 Me, 46 \pm 3, 42-3.5°, 54 \pm 3, 87, b₂ 141-2°; iso-Pr,
 Me, 53 \pm 3, 36-7°, 47 \pm 3, 86, b₃ 124.5-6-5°; and Ph,
 Et (II), 77 \pm 5, 79°, 23 \pm 5, 87, -. The configuration of threo-II was determined by comparison with an authentic sample. The configuration of threo-I was proved by reduction of the compound with LiAlH₄ to a β -diol, which was identical with the compound obtained by transformation of trans- α -methylcinnamic acid into the corresponding ethylenic alc., followed by hydroboration of the alc. Nuclear magnetic resonance spectra were used to determine the configurations of the other stereoisomers. Possible intermediates in the Reformatskii reaction are discussed.

IT 17226-93-6, Hydracrylic acid, 2,3-diphenyl-, methyl ester, threo-

17226-94-7, Hydracrylic acid, 2,3-diphenyl-, methyl ester,

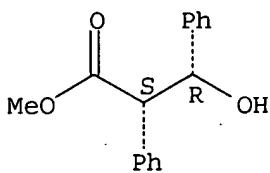
erythro-

(preparation of)

RN 17226-93-6 CAPLUS

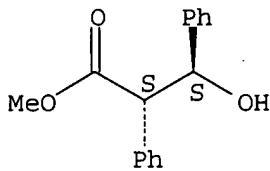
CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
(α R, β S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 17226-94-7 CAPLUS
 CN Benzenepropanoic acid, β -hydroxy- α -phenyl-, methyl ester,
 (α R, β R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L15 ANSWER 57 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1963:461744 CAPLUS
 DN 59:61744
 OREF 59:11299d-h,11300a-d
 TI Analgesics. Absolute configuration of α -(+)-4-dimethyl-amino-1,2-diphenyl-3-methyl-2-propionoxybutane, d-propoxyphene
 AU Sullivan, H. R.; Beck, J. R.; Pohland, A.
 CS Eli Lilly & Co., Indianapolis, IN
 SO Journal of Organic Chemistry (1963), 28(9), 2381-5
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA Unavailable
 GI For diagram(s), see printed CA Issue.
 AB α -(+)-Me₂NCH₂CHMeCPh(CH₂Ph)O₂C₂H₅.HCl (I) (15 g.) and 135 mL. 5N HCl was refluxed 2 h. and concentrated to dryness to give 8.5 g. (--)Me₂NCH₂CHMeCPh:CHPh.HCl (II), m. 189-90° (MeOH-EtOAc), $[\alpha]$ (all 25/D) -33.7° (c 1, H₂O). Similarly, 50 g. α -(-) isomer of I gave 21 g. II (--) isomer (III), m. 189-90°, $[\alpha]$ 34.3° (c 1, H₂O). Into 25 g. II, 150 mL. MeOH, and 1100 mL. EtOAc at -20° was passed O₃ in excess; the whole added to 250 mL. ice-H₂O, kept overnight, the MeOH and EtOAc distilled in vacuo, the aqueous solution washed with Et₂O (concentration of these gave BzH), the aqueous solution treated with excess aqueous NH₃, extracted with Et₂O, and the Et₂O, exts. dried and treated with dry HCl gave 8 g. (--)Me₂NCH₂CHMeBz.HCl (IV), m. 153-4° (MeOH-EtOAc), $[\alpha]$ -47° (c 1, H₂O). To 11.8 g. IV, 130 g. anhydrous Na₂HPO₄, and 300 mL. CH₂Cl₂ at 0-5° was added CF₃-CO₂H [from 50.8 g. (CF₃CO)₂O, 8.2 mL. 90% H₂O₂, and 100 mL. CH₂Cl₂, at 0°]; the whole stirred 1 h. (temperature rise to 10°), the solid mixture kept 4 h. at room temperature, 200 mL. H₂O added, the CH₂Cl₂ phase separated, evaporated to dryness, the residue dissolved in 100 mL. 2N HCl, washed, treated with excess concentrated aqueous NH₃ and extracted with Et₂O and the dried Et₂O solution treated with dry HCl gave 3.8 g. (--)Me₂NCH₂CHMeOBz.HCl, m. 160-1° (MeOH-EtOAc), $[\alpha]$ -62.8° (c 1, H₂O). D(-)-H₂NCH₂CH- (OH)Me.HCl (2.7 g.), 1.6 g. HCO₂Na, 8.3 g. 100% HCO₂H, and

6.7 g. 37% HCHO were refluxed 14 h. to give 3.13 g. hygroscopic D(--)-Me₂NCH₂CH(OH)Me.HCl (V), $[\alpha]$ -44.5° (c 1, MeOH); V, 7.1 g. BzCl, 25 mL. Et₃N, and 80 mL. CHCl₃ refluxed 1 h. gave 4.2 g. Me₂NCH₂CH(OBz)Me, HCl, m. 160-1° (MeOH-EtOAc), $[\alpha]$ -63.3° (c 1, H₂O). I (370 g.), 4.5 l. MeOH, and 650 mL. 30% H₂O₂ kept 48 h. at room temperature, the whole evaporated to dryness, 0.4 g. PtO₂ added

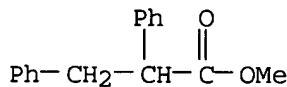
(caution), filtered, the filtrate evaporated to dryness, and the residue in 2 l. EtOAc treated with 40 g. HCl in 1 l. EtOAc gave 370 g. I N-oxide-HCl (VI), m. 186-7° (MeOH EtOAc), $[\alpha]$ 20.2° (c 2, MeOH); VI in 1500 mL. H₂O saturated with K₂CO₃ and extracted with Et₂O gave 320 g. N-oxide (VII); VII heated slowly at 0.5 mm. to 140°, kept 0.5 h. at 140°, the whole cooled, dissolved in Et₂O and the Et₂O solution washed, dried, concentrated and distilled gave 200 g. (+)-CH₂:CMeCPh(CHPh)O₂CET (VIII), b_{0.6} 152°, n_{25D} 1.5466, $[\alpha]$ 97° (c 1.3, Me₂CO) (the cold trap from the pyrolysis contained Me₂NHOH). VIII (45 g.) in 1 l. EtOAc at -50° and O₃ to blue color, the whole poured into ice-H₂O, kept overnight, dilute aqueous NaHSO₃ added, dropwise, to neg. starch-iodide test, the EtOAc solution separated, washed and dried gave 41 g. (+)-AcCPh-(O₂CET)CH₂Ph (IX), b_{0.5} 156-7°, $[\alpha]$ 182.7° (c 1.1, Me₂CO). IX (32.5 g.), 1 l. 5N HCl, and 1 l. EtOH refluxed 20 h. gave 21.9 g. (+)-AcC(OH)PhCH₂Ph (X), b_{0.5} 148°, n_{25D} 1.5660, $[\alpha]$ 141° (c 1.3, EtOH). To 60 g. X in 200 mL. glacial AcOH was added, dropwise, 45 g. Br in 100 mL. glacial AcOH, and the whole stirred 1 h. and evaporated to dryness in vacuo; the residue in 600 mL. C₅H₅N heated 1 h. at 100°, the whole concentrated, and the residue and 60 g. NaOH in 900 mL. H₂O heated 2 h. at 100° gave 20 g. (-)-PhCH₂C(OH)PhCO₂H (XI), m. 145-6° (aqueous EtOH), $[\alpha]$ 13.7° (c 3.5, EtOH). XI (18 g.), 40 g. Ag₂O and 200 mL. MeI refluxed and stirred 3 h. gave 15 g. Me ester (XII), m. 102-3° (Et₂O-petr. ether), $[\alpha]$ -32.4° (c 3.4, CHCl₃). Absolute EtOH, (200 mL.) and 60 g. freshly prepared W-2 Raney Ni, shaken first with 40 lb./in.² H, 8 g. XII added, and the whole refluxed 8 h., filtered, the residue from the concentration of the filtrate dissolved in 40 mL. petr. ether, 1.4 g. XII which separated, filtered off, the filtrate evaporated and the residue

distilled gave 6 g. (+)-PhCH₂CHPhCO₂Me (XIII), b_{0.2} 123-4°, n_{25D} 1.5518, $[\alpha]$ -90.5° (c 4.6, CHCl₃). To 1.7 g. LiAlH₄ in 110 mL. anhydrous Et₂O was added 10.2 g. XIII in 40 mL. Et₂O, dropwise, and the whole refluxed 3 h. to give 7.8 g. (+)-PhCH₂CHPhCH₂OH, b_{0.2} 128°, n_{25D} 1.5742, $[\alpha]$ 76.3°; tosylate (XIV) (prepared in C₅H₅N), m. 89-90° (Me₂CO-petr. ether), $[\alpha]$ 40.2° (c 2.4, Me₂CO). XIV (7.4 g.), 16.5 g. NaI, and 200 mL. anhydrous Me₂CO refluxed and stirred 20 h. gave 6.35 g. (+)-PhCH₂CHPhCH₂I (XV), m. 54-5° (petr. ether), $[\alpha]$ 16.6° (c 3.9, EtOH); XV, 3.0 g. NaHCO₃, 150 mL. absolute EtOH, and 5 g. Pd-C hydrogenated 10 h. at 25° gave 2.6 g. (+)-PhCH₂CHPhMe, b_{0.3} 85°, n_{25D} 1.5558, $[\alpha]$ 76.7° (c 2.3, CHCl₃). (-)-threo-PhCH(OH)CHPhMe (1.4 g.) added to 100 mL. absolute EtOH and 30 g. W-2 Raney Ni, shaken first in H as above, and the whole refluxed 8 h. gave 1.15 g. D(-)-PhCH₂CHPhMe, b_{0.5} 88°, n_{25D} 1.5553, $[\alpha]$ -76.3° (c 2.2, CHCl₃). The absolute configuration of I is (2S.3R).

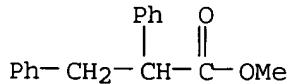
IT 35030-49-0, Propionic acid, 2,3-diphenyl-, methyl ester
(preparation of)

RN 35030-49-0 CAPLUS

CN Benzenepropanoic acid, α -phenyl-, methyl ester (9CI) (CA INDEX
NAME)



L15 ANSWER 58 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1962:462469 CAPLUS
 DN 57:62469
 OREF 57:12373g-h
 TI Relative signs of geminal and vicinal proton-proton coupling constants in α,β -diphenylpropionic acid and its methyl ester
 AU Fraser, Robert R.
 CS Univ. Ottawa
 SO Canadian Journal of Chemistry (1962), 40, 1483-9
 CODEN: CJCHAG; ISSN: 0008-4042
 DT Journal
 LA Unavailable
 AB Since theoretical calcns. of vicinal coupling consts. and geminal coupling consts. predicted the same sign as long as the bond angle between the geminal hydrogens is less than 125°; it has now been shown that geminal and vicinal consts. are opposite in sign in α,β -diphenylpropionic acid (I) and its Me ester (II). The spectrum of I measured at 60 Mc./sec. shows 11 transitions. The spectrum of II shows 13. A tabulation of intensities and spectra at other frequencies is listed.
 IT 35030-49-0, Propionic acid, 2,3-diphenyl-, methyl ester
 (nuclear magnetic resonance and spin-spin coupling of)
 RN 35030-49-0 CAPLUS
 CN Benzenepropanoic acid, α -phenyl-, methyl ester (9CI) (CA INDEX
 NAME)



=>